



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 01:07 AM EDT

PDB ID : 6ERP
Title : Structure of the human mitochondrial transcription initiation complex at the LSP promoter
Authors : Hillen, H.S.; Morozov, Y.I.; Sarfallah, A.; Temiakov, D.; Cramer, P.
Deposited on : 2017-10-18
Resolution : 4.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

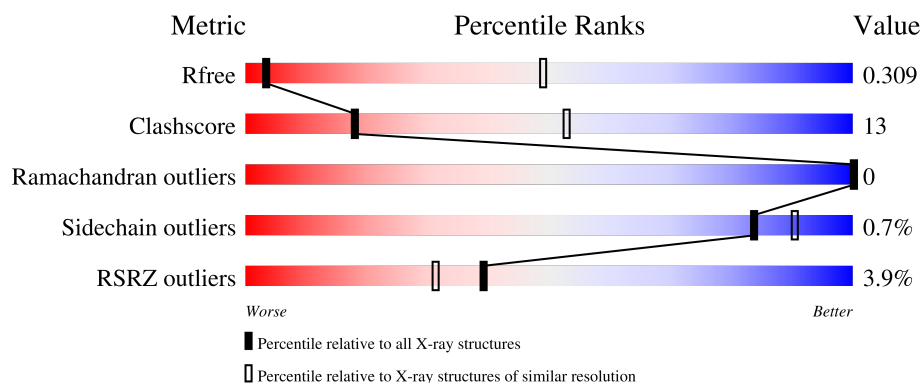
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	205	<div> <div>5%</div> <div>67%</div> <div>26%</div> <div>6%</div> </div>
1	G	205	<div> <div>7%</div> <div>71%</div> <div>22%</div> <div>6%</div> </div>
2	D	50	<div> <div>2%</div> <div>26%</div> <div>64%</div> <div>8%</div> </div>
2	H	50	<div> <div>2%</div> <div>54%</div> <div>38%</div> <div>8%</div> </div>
3	E	50	<div> <div>2%</div> <div>22%</div> <div>64%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	50	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>26%</div><div>60%</div><div>10%</div></div><div><div></div><div></div><div></div></div></div>
4	A	1128	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>67%</div><div>22%</div><div>10%</div></div><div><div></div><div></div><div></div></div></div>
4	B	1128	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>20%</div><div>11%</div></div><div><div></div><div></div><div></div></div></div>
5	F	377	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>58%</div><div>19%</div><div>24%</div></div><div><div></div><div></div><div></div></div></div>
5	J	377	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>59%</div><div>17%</div><div>24%</div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27644 atoms, of which 42 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			
1	G	192	Total	C	N	O	S	0	0	0
			1615	1019	291	300	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	41	ASN	-	expression tag	UNP Q00059
C	42	ALA	-	expression tag	UNP Q00059
C	49	SER	CYS	conflict	UNP Q00059
G	41	ASN	-	expression tag	UNP Q00059
G	42	ALA	-	expression tag	UNP Q00059
G	49	SER	CYS	conflict	UNP Q00059

- Molecule 2 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			
2	H	46	Total	C	N	O	P	0	0	0
			952	454	176	277	45			

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			
3	I	45	Total	C	N	O	P	0	0	0
			907	434	163	266	44			

- Molecule 4 is a protein called DNA-directed RNA polymerase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1011	Total	C	N	O	S	0	0	0
			8028	5107	1452	1418	51			
4	B	1003	Total	C	N	O	S	0	0	0
			7974	5073	1444	1406	51			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	-	expression tag	UNP O00411
A	104	ALA	-	expression tag	UNP O00411
A	555	ALA	GLU	engineered mutation	UNP O00411
B	103	ASN	-	expression tag	UNP O00411
B	104	ALA	-	expression tag	UNP O00411
B	555	ALA	GLU	engineered mutation	UNP O00411

- Molecule 5 is a protein called Dimethyladenosine transferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	288	Total	C	H	N	O	S	0	0
			2347	1506	21	397	408	15		
5	J	288	Total	C	H	N	O	S	0	0
			2347	1506	21	397	408	15		

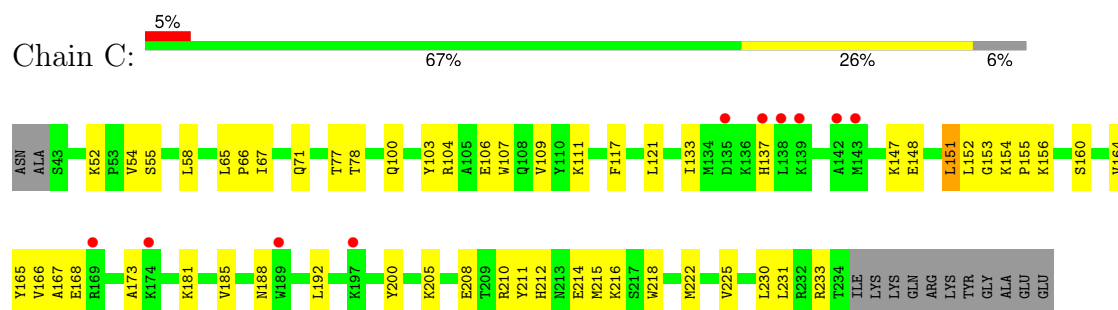
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	20	ASN	-	expression tag	UNP Q9H5Q4
F	21	ALA	GLY	conflict	UNP Q9H5Q4
J	20	ASN	-	expression tag	UNP Q9H5Q4
J	21	ALA	GLY	conflict	UNP Q9H5Q4

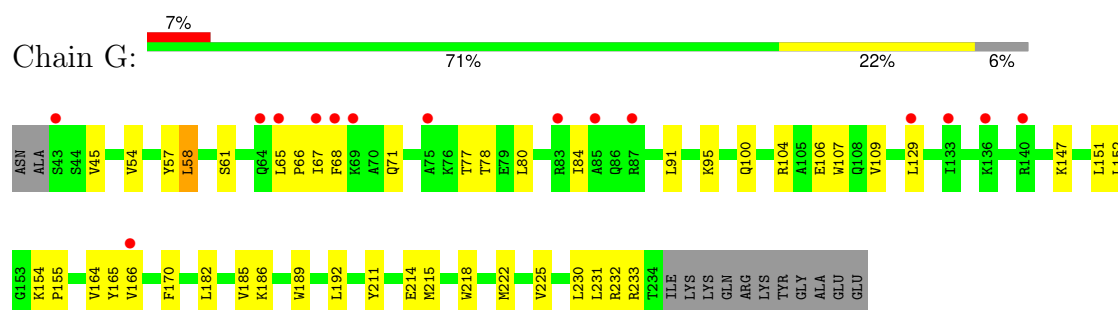
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

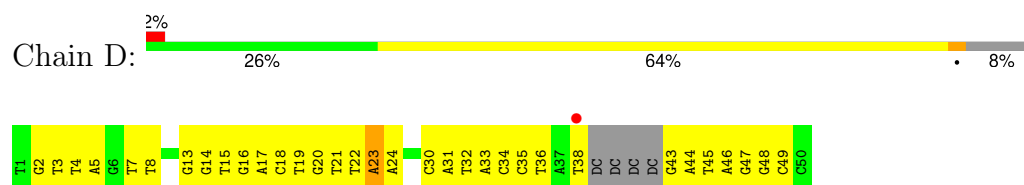
- Molecule 1: Transcription factor A, mitochondrial



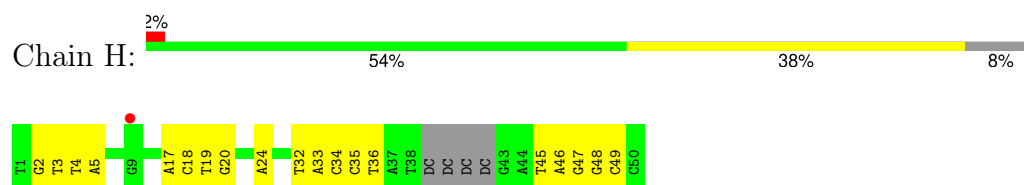
- Molecule 1: Transcription factor A, mitochondrial



- Molecule 2: Non-Template DNA



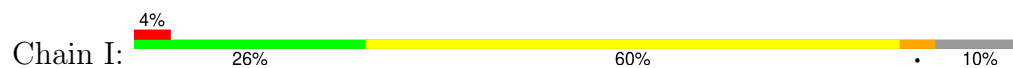
- Molecule 2: Non-Template DNA



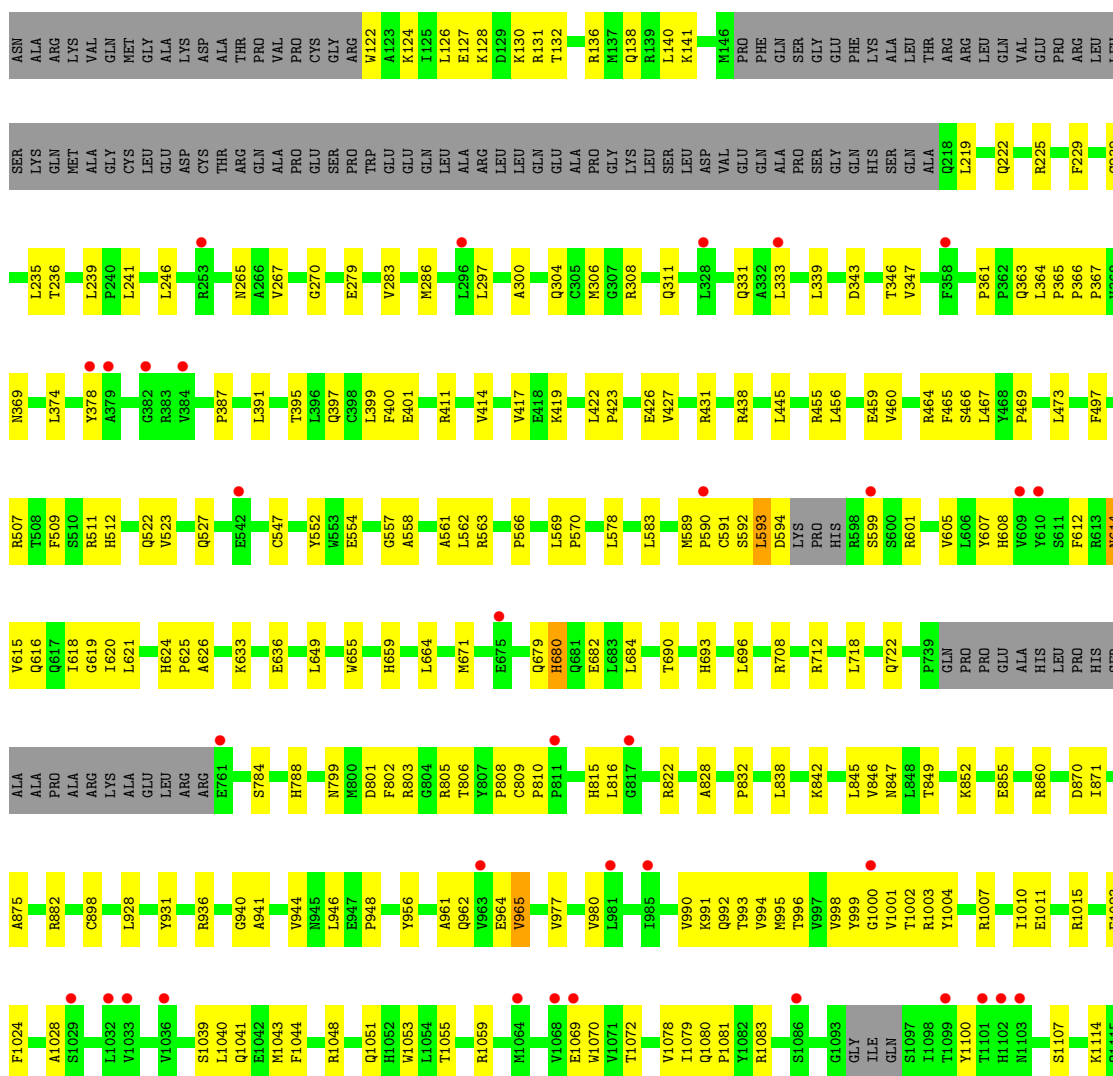
- Molecule 3: Template DNA



• Molecule 3: Template DNA

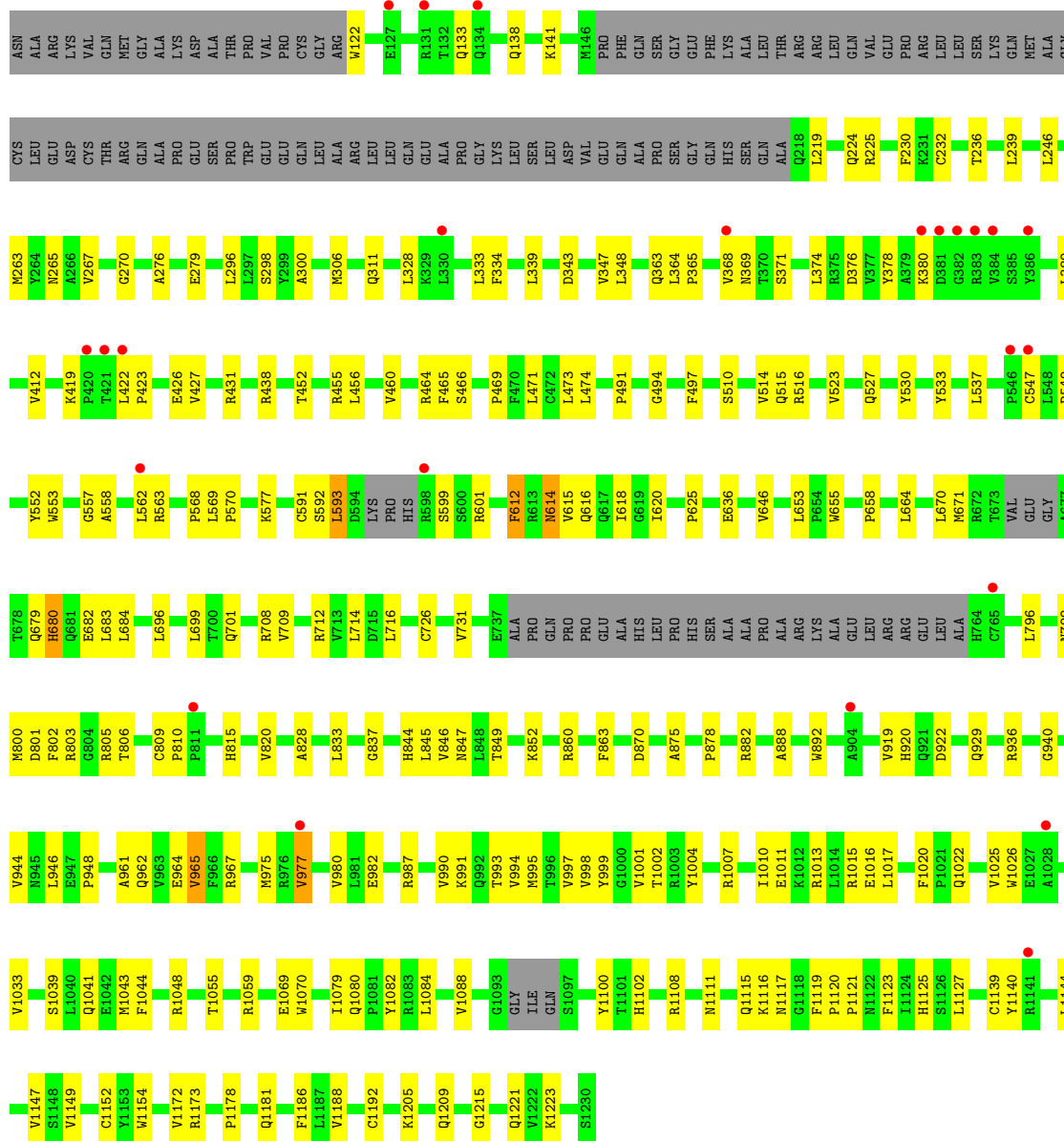


• Molecule 4: DNA-directed RNA polymerase, mitochondrial

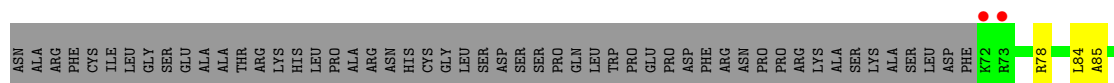


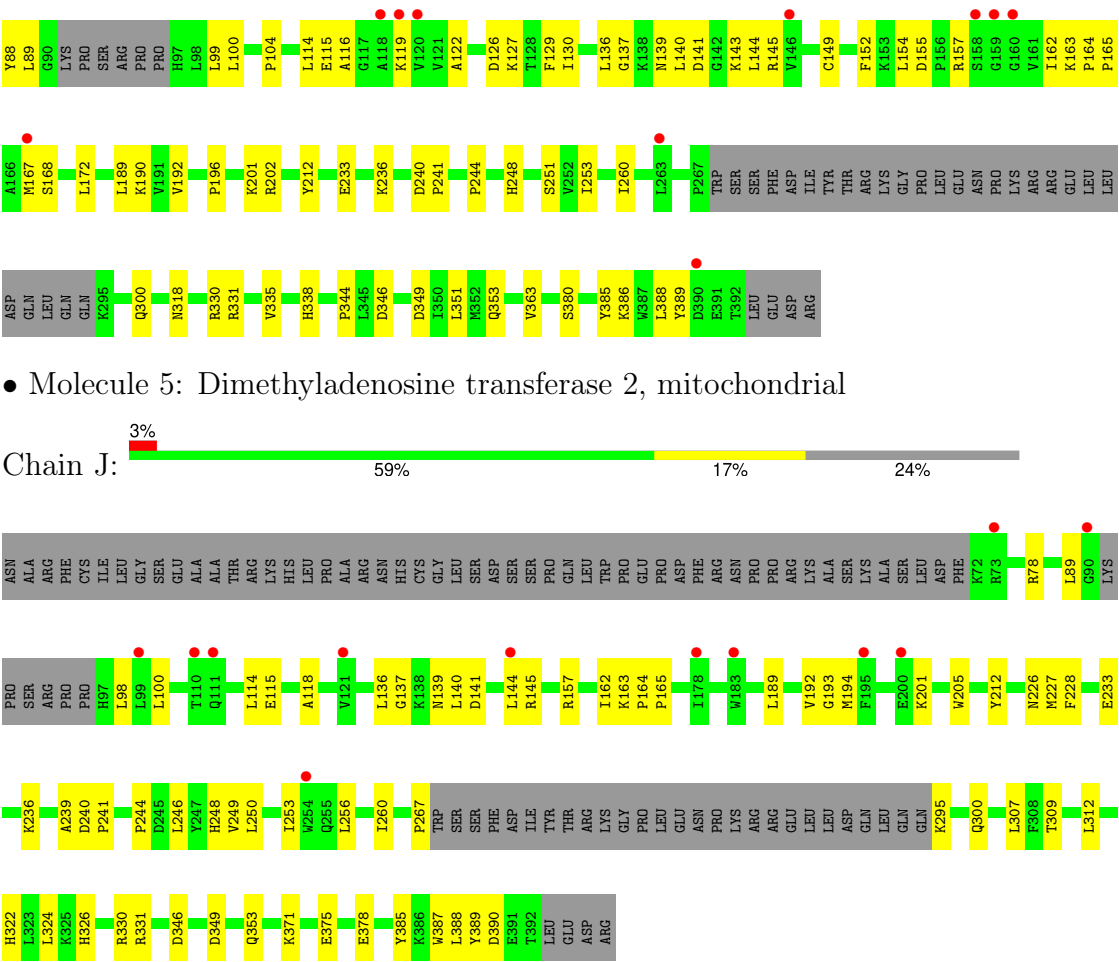


• Molecule 4: DNA-directed RNA polymerase, mitochondrial



• Molecule 5: Dimethyladenosine transferase 2, mitochondrial





● Molecule 5: Dimethyladenosine transferase 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 197.03Å 137.21Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	49.58 – 4.50 49.58 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.58-4.50) 98.8 (49.58-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.270 , 0.310 0.272 , 0.309	Depositor DCC
R_{free} test set	1595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	276.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 290.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	27644	wwPDB-VP
Average B, all atoms (Å ²)	379.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	C	0.23	0/1646	0.35	0/2202
1	G	0.23	0/1646	0.36	0/2202
2	D	0.51	0/1068	0.95	1/1648 (0.1%)
2	H	0.53	0/1068	0.96	0/1648
3	E	0.57	0/1014	1.06	4/1557 (0.3%)
3	I	0.57	0/1014	1.05	4/1557 (0.3%)
4	A	0.23	0/8213	0.38	0/11132
4	B	0.23	0/8157	0.39	0/11053
5	F	0.24	0/2380	0.38	0/3213
5	J	0.23	0/2380	0.38	0/3213
All	All	0.30	0/28586	0.54	9/39425 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	20	DT	OP1-P-OP2	11.64	137.06	119.60
3	I	20	DT	OP1-P-OP2	11.11	136.27	119.60
3	E	19	DA	OP2-P-O3'	-10.97	81.06	105.20
3	I	19	DA	OP2-P-O3'	-10.76	81.54	105.20
3	E	19	DA	OP1-P-O3'	-9.04	85.32	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1615	0	1655	55	0
1	G	1615	0	1655	46	0
2	D	952	0	523	36	0
2	H	952	0	523	19	0
3	E	907	0	508	63	0
3	I	907	0	508	52	0
4	A	8028	0	8092	209	0
4	B	7974	0	8039	198	0
5	F	2326	21	2375	63	0
5	J	2326	21	2375	51	0
All	All	27602	42	26253	725	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 725 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:363:GLN:HB3	4:B:364:LEU:HG	1.28	1.13
4:A:363:GLN:HB3	4:A:364:LEU:HG	1.34	1.07
4:B:975:MET:HE2	4:B:977:VAL:HG23	1.31	1.04
1:G:152:LEU:HD21	1:G:230:LEU:HD13	1.41	1.02
5:F:89:LEU:HD11	5:F:116:ALA:HB1	1.42	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	190/205 (93%)	184 (97%)	6 (3%)	0	100	100
1	G	190/205 (93%)	187 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1001/1128 (89%)	962 (96%)	39 (4%)	0	100	100
4	B	991/1128 (88%)	958 (97%)	33 (3%)	0	100	100
5	F	282/377 (75%)	271 (96%)	11 (4%)	0	100	100
5	J	282/377 (75%)	272 (96%)	10 (4%)	0	100	100
All	All	2936/3420 (86%)	2834 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	178/188 (95%)	177 (99%)	1 (1%)	86	92
1	G	178/188 (95%)	177 (99%)	1 (1%)	86	92
4	A	865/976 (89%)	859 (99%)	6 (1%)	84	90
4	B	860/976 (88%)	853 (99%)	7 (1%)	81	89
5	F	255/335 (76%)	254 (100%)	1 (0%)	91	94
5	J	255/335 (76%)	253 (99%)	2 (1%)	81	89
All	All	2591/2998 (86%)	2573 (99%)	18 (1%)	84	90

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	1108	ARG
5	J	388	LEU
5	J	157	ARG
4	B	593	LEU
4	B	977	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	363	GLN
4	B	969	GLN
4	B	893	GLN
4	B	1063	HIS
4	A	722	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	192/205 (93%)	0.02	10 (5%) 27 24	312, 394, 446, 483	0
1	G	192/205 (93%)	0.23	15 (7%) 13 11	405, 477, 524, 533	0
2	D	46/50 (92%)	-0.17	1 (2%) 62 52	337, 410, 526, 562	0
2	H	46/50 (92%)	-0.02	1 (2%) 62 52	415, 474, 534, 545	0
3	E	45/50 (90%)	-0.16	1 (2%) 62 52	359, 433, 502, 518	0
3	I	45/50 (90%)	-0.05	2 (4%) 34 28	413, 483, 558, 625	0
4	A	1011/1128 (89%)	0.16	45 (4%) 33 28	246, 329, 411, 462	0
4	B	1003/1128 (88%)	0.05	24 (2%) 59 49	269, 356, 432, 478	0
5	F	288/377 (76%)	-0.04	12 (4%) 36 30	287, 345, 461, 501	0
5	J	288/377 (76%)	0.07	12 (4%) 36 30	325, 411, 582, 648	0
All	All	3156/3620 (87%)	0.08	123 (3%) 39 31	246, 362, 500, 648	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	38	DT	5.7
4	A	379	ALA	5.6
4	A	358	PHE	5.6
3	I	14	DG	5.1
4	B	384	VAL	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.